Realizations of Magnetic-Monopole Gauge Fields: Diatoms and Spin Precession

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It is found that the effective Hamiltonian for nuclear rotation in a diatom is equivalent to that of a charged particle in a background magnetic-monopole field. In certain cases, half-integer orbital angular momentum or non-Abelian fields occur. Furthermore, the effects of magnetic-monopole-like gauge fields can be experimentally observed in spin-resonance experiments with variable magnetic fields.

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Gauge potentials have been found to appear very naturally in the description of quantum-mechanical systems which depend upon slowly varying external parameters. Berry[1] performed a detailed study of Abelian potentials which appear when a single nondegenerate level is subjected to adiabatically varying external parameters. He showed that Abelian magnetic-monopole fields can occur near a degeneracy of the quantum levels (the monopole) in the space of external parameters. He also proposed an interference experiment using split electron beams to search for an "excess" geometrical phase induced by his gauge potentials. Simon[2] recast Berry's findings in the language of holonomy theory and made a connection to the quantum Hall effect. Finally, Wilczek and Zee[3] showed that non-Abelian gauge potentials can arise when sets of degenerate levels are subjected to adiabatically varying external parameters.

In work preceding Berry's by over twenty years, Herzberg and Longuet-Higgins[4] noticed sign ambiguities in the Born-Oppenheimer[5] wave functions of simple molecules. These sign ambiguities are associated with conical intersections in the zeroth-order electronic energy levels. To compensate for these and other, more general, phase ambiguities and thus to make the Born-Oppenheimer wave functions single valued, Mead[6] suggested adding a "vector-potential-type term" to the nuclear Hamiltonian. He refers to the effects of this term on the nuclear motion as the molecular Bohm-Aharonov effect.

The gauge potentials of Berry, Simon, and Wilczek and Zee can be generalized to systems where the slowly varying parameters are no longer external, but are themselves quantized; in the case of molecular physics, these are the nuclear coordinates. Such a description subsumes the findings of Herzberg and Longuet-Higgins and Mead. In a paper to be published elsewhere,[7] we show that the Born-Oppenheimer description of molecules can be cast in a rigorously gauge-covariant form, and discuss higher-order corrections to this description.

Diatoms as monopoles.—In the Born-Oppenheimer method,[5,7] eigenfunctions of the full Hamiltonian

$$H(R,r) = -\frac{1}{2m_N}\nabla_R^2 - \frac{1}{2m_e}\nabla_r^2 + V_N(R) + V_e(R,r) \tag{1}$$

are decomposed into electric and nuclear components:

$$\Psi^a(R,r) = \sum_m \Phi_m^a(R)\phi_m(R,r).$$

Here R and r are nuclear and electronic coordinates, respectively. The $\phi_m(R,r)$ form a basis of electronic eigenfunctions of H for fixed R when the nuclear kinetic energy term is ignored; the energy of the state $\phi_m(R,r)$ is denoted by $\epsilon_m(R)$. The vector wave functions Φ_m^a are then acted on by the matrix-valued nuclear Hamiltonian H_{mn} which results when H is sandwiched between electronic eigenstates $|n(R)\rangle = |\phi_n\rangle$:

$$H_{mn} = -\frac{1}{2m_N}\sum_l [\nabla_R + \langle m(R)|\nabla_R|l(R)\rangle][\nabla_R + \langle l(R)|\nabla_R|n(R)\rangle] + V_N(R)\delta_{mn} + \epsilon_n(R)\delta_{mn}. \tag{2}$$

Here, H_{mn} is exact and has been written in gauge-covariant form.[8] The $\epsilon_n(R)$ act as effective potentials for the nuclear motion, while the $\langle m|\nabla_R|n\rangle$ act as effective gauge potentials and transition terms between different electronic states. In the adiabatic limit, where the nuclei move very slowly relative to the electrons, we may assume that the electrons remain in the nth level [i.e., we ignore off-diagonal transition terms in (2)], in which case the relevant Hamiltonian is approximately

$$H_n^{\text{eff}} \simeq -\frac{1}{2m_N}[\nabla_R - i\mathbf{A}(R)]^2 + V'(R), \tag{3}$$

where $\mathbf{A}(R) = \langle n|i\nabla_R|n(R)\rangle$. As noted by Mead[6] and Berry[1] and discussed in detail in Ref. 7, $\mathbf{A}$

transforms as a U(1) gauge potential when we locally change our choice of phases for $|n(R)\rangle$. If $|n\rangle$ belongs to an N-fold degenerate level, $\mathbf{A}$ is an $N\times N$ matrix which transforms as a U(N) gauge potential.[3,7] The approximation leading to (3) differs from the usual Born-Oppenheimer approximation where $|n(R)\rangle$ is chosen real so that $\mathbf{A}(R)=0$. As we shall see, this choice of gauge is not always possible globally.

For example, we consider the doubly degenerate Λ levels of a diatomic molecule. The effective Hamiltonian for this system is, in general, a 2×2 non-Abelian matrix determined as follows. Given the electronic eigenstates with $\Lambda=\pm l$ for the nuclear axis in the $\theta=\phi=0$ direction, we can choose a family of eigenstates adapted to nuclei pointing toward θ,ϕ by simple rotations:

$$|\pm(\theta,\phi)\rangle = e^{iJ_3\phi}e^{iJ_1\theta}e^{-iJ_3\phi}|\pm(0,0)\rangle. \tag{4}$$

According to our general prescription one then finds effective U(2) gauge potentials which are 2×2 matrices (with $\pm$ indices implicit):

$$A_\theta = \langle\theta,\phi|i\partial/\partial\theta|\theta,\phi\rangle = \langle 0,0|-e^{iJ_3\phi}J_1e^{-iJ_3\phi}|0,0\rangle = \langle 0,0|[-\cos\phi J_1+\sin\phi J_2]|0,0\rangle, \tag{5}$$

$$A_\phi = \langle\theta,\phi|i\partial/\partial\phi|\theta,\phi\rangle = \langle 0,0|[(1-\cos\theta)J_3+\sin\theta\sin\phi J_1+\sin\theta J_2]|0,0\rangle. \tag{6}$$

If $l\neq\frac{1}{2}$ we find $A_\theta=0$. A_ϕ is also readily evaluated in this case; one finds an "Abelianized" diagonal structure

$$A_\phi^{++}=l(1-\cos\theta),\quad A_\phi^{--}=-l(1-\cos\theta),\quad A_\phi^{+-}=A_\phi^{-+}=0. \tag{7}$$

More compactly, we may write $A_\phi=l(1-\cos\theta)\sigma_3$. Evaluating the field strength one finds $F_{\theta\phi}=\partial_\theta A_\phi-\partial_\phi A_\theta=l\sin\theta\sigma_3$, or for the corresponding Cartesian tensor $[F_{\theta\phi}\equiv(g^{\theta\theta})^{1/2}(g^{\phi\phi})^{1/2}]$ on the sphere simply

$$\hat{F}_{\theta\phi}=l\sigma_3. \tag{8}$$

Evidently, the nuclear coordinates act as if they parametrize the motion of a charged particle in a magnetic-monopole field.

To analyze this further, we need the angular momentum operators appropriate to the problem.[9] They are

$$\tilde{J}_x = i\left\{\sin\phi\frac{\partial}{\partial\theta}+\cot\theta\cos\phi\frac{\partial}{\partial\phi}\right\}-l\frac{1-\cos\theta}{\sin\theta}\cos\phi\,\sigma_3,$$
$$\tilde{J}_y = i\left\{-\cos\phi\frac{\partial}{\partial\theta}+\cot\theta\sin\phi\frac{\partial}{\partial\phi}\right\}-l\frac{1-\cos\theta}{\sin\theta}\sin\phi\,\sigma_3,\quad \tilde{J}_z = i\left\{-\frac{\partial}{\partial\phi}\right\}-l\sigma_3, \tag{9}$$

where in each case the bracketed term is the standard or naive rotation operator. $\tilde{J}$ may be rewritten in the more compact form

$$\tilde{\mathbf{J}} = -i\mathbf{r}\times\mathbf{D}-\tfrac{1}{2}\mathbf{r}\epsilon_{ijk}r_iF_{jk}, \tag{10}$$

where $\mathbf{D}=\nabla-i\mathbf{A}$. Note that half-integer angular momentum is associated with the *orbital* nuclear motion, for l half integer.[10]

We may now write the Hamiltonian (1) as

$$H=\tfrac{1}{2}(\tilde{J}^2-l^2),$$

and construct its eigenstates by the usual procedure.[10]

The truly non-Abelian case $l=\frac{1}{2}$.—Although the algebra starting from Eq. (7) does not especially distinguish the case $l=\frac{1}{2}$, the original physical problem *is* different for this case. Specifically, in evaluating the potentials (5) and (6) we find off-diagonal terms:

$$A_\theta=\tfrac{1}{2}\begin{pmatrix}0 & -\kappa e^{i\phi}\\ -\kappa e^{-i\phi} & 0\end{pmatrix}, \tag{11}$$

$$A_\phi=\tfrac{1}{2}\begin{pmatrix}1-\cos\theta & -i\kappa e^{i\phi}\sin\theta\\ i\kappa e^{-i\phi}\sin\theta & -1+\cos\theta\end{pmatrix}, \tag{12}$$

where $\kappa=2\langle+|J_1|-\rangle$. Since the states in question are not eigenfunctions of angular momentum (but only of J_3), κ can in principle take any value; we have taken it real without loss of generality. From (11) and (12) we compute the field strength

$$F_{\theta\phi}=\partial_\theta A_\phi-\partial_\phi A_\theta-i[A_\theta,A_\phi]$$
$$=\tfrac{1}{2}(1-\kappa^2)\sin\theta\,\sigma_3. \tag{13}$$

The field strength (13) vanishes for $\kappa=1$. This might have been anticipated, for the following reason: If the degenerate electron states with $\Lambda=\pm\frac{1}{2}$ actually formed a representation of the rotation group we would have $\kappa=1$. Furthermore, we could choose a fixed basis for the electron states, independent of the nuclear-axis orientation, since the two-dimensional *space* of states is rotationally invariant.

The field strength (13) superficially resembles the monopole field (8) that we encountered before, but the interpretation here is quite different. For one thing, κ is not quantized. At a deeper level, in the present case the gauge fields are *truly non-Abelian* (for

$\kappa \neq \pm 1$). While previously the potentials (7) all pointed in the same direction in internal space, here they do not. It is important to check that they cannot be made to do so by a different choice of basis, i.e., in a different gauge. Actually this already follows from the fact that the field strength is not quantized; it can also be seen by noting that the covariant derivative of the field strength, $D_\phi F_{\theta\phi}$, has a contribution from the commutator, which implies that it does *not* point in the same direction as $F_{\theta\phi}$ in internal space.

Because of the nonvanishing of $D_\phi F_{\theta\phi}$, the operators of Eq. (10) do not satisfy the angular momentum commutation relations. However, the "Abelianized" operators appropriate to the $\kappa = 0$ case, i.e., Eq. (9) with $l = \frac{1}{2}$, commute with the Hamiltonian not only for $\kappa = 0$ but generally. We do not know of a canonical procedure which yields these angular momentum operators, but we are convinced of their uniqueness (for $\kappa \neq \pm 1$). There is no nontrivial κ dependence which may be added to the operators of Eq. (10) that preserves their algebra.[11]

The implications of the equation implying conservation of $\tilde{J}$,

$$[\tilde{J}_i, H_\kappa - H_0] = 0, \tag{14}$$

can be made more transparent by defining the block-diagonal operators

$$\tilde{J}_i = \begin{pmatrix} M_i & 0 \\ 0 & N_i \end{pmatrix}, \quad H_\kappa - H_0 = \kappa \begin{pmatrix} 0 & C \\ C^* & 0 \end{pmatrix} + \frac{\kappa^2}{2}. \tag{15}$$

Here M_i and N_i each satisfy the angular momentum algebra, and (14) gives the intertwining relations

$$M_i C = C N_i, \quad C^* M_i = N_i C^*. \tag{16}$$

A direct computation gives

$$\begin{pmatrix} 0 & C \\ C^* & 0 \end{pmatrix}^2 = \tilde{J}^2 + \tfrac{1}{4}. \tag{17}$$

Thus C is a sort of a Dirac operator, roughly a local square root of the covariant spherical Laplacian. Its effect is to split the eigenvalues of H by $2\kappa(j + \frac{1}{2})$, in agreement with the classic result.[12]

Spin precession in an oscillating magnetic field.—In the preceding section, we saw how magnetic-monopole fields can arise dynamically in the context of the Born-Oppenheimer method. Berry studied the case of spins in an applied, adiabatically varying magnetic field and found another monopole, leading to a nondynamical precession effect. He showed that if the external magnetic field goes around a closed path $B(t)$ $(0 \leq t \leq T)$ enclosing a solid angle Ω, then spin-$\frac{1}{2}$ wave functions with $s_z = \pm \frac{1}{2}$ acquire geometrical phases $\exp(\pm i\Omega/2)$ in addition to the dynamical phase $\exp[-i\int_0^T E(t)\,dt]$. The relative phase between the two spin components implies an extra rotation of the spin by an angle Ω in the x-y plane. In B space, this mimics the effect of a magnetic monopole at $B = 0$ with unit Dirac charge on electrically charged particles following the trajectory $B(t)$. Berry proposed an experiment to observe this geometric phase by splitting an electron beam in a magnetic field, rotating the field applied to one of the components of the beam, and looking for interference when the split beam is recombined. Unfortunately, such an experiment is impractical, because of the difficulty in guaranteeing identical dynamical evolution of the two beam components.

We wish to point out that Berry's result may be extended to the case of spins in a rapidly oscillating magnetic field, thus providing a practical way to measure geometric phases within the familiar context of magnetic resonance. Specifically, let B_z be a large constant orienting field and $B_\perp(t)\sin(\omega t)$ a small, slowly modulated oscillating field with mean rf frequency ω in the x-y plane. Then regarding $B_\perp$ and ω as free parameters and varying $B_\perp$ around a closed loop will result in a geometric phase which can be observed by beating the resulting rf signal against a reference signal. Thus, an interference experiment is done upon a single sample, avoiding the problem of guaranteeing precisely equivalent dynamical evolution for two separate systems.

Consider the Hamiltonian

$$H_{\text{lab}} = -\gamma\boldsymbol{\sigma} \cdot [B_z \hat{\mathbf{z}} + \mathbf{B}_\perp(t)\sin\omega t]. \tag{18}$$

We suppose operation near a resonant frequency $\omega \approx \omega_0 = \gamma B_z$, and go to the rotating frame. The appropriate effective Hamiltonian is

$$H_{\text{rot}} = -\gamma\boldsymbol{\sigma} \cdot \left[B_z \left(1 - \frac{\omega}{\omega_0} \right) \hat{\mathbf{z}} + \mathbf{B}_\perp(t) \right]. \tag{19}$$

This is precisely the sort of Hamiltonian considered by Berry, with the origin (and the monopole) now located at the resonance point $\omega = \omega_0$, $B_\perp = 0$. Thus a variation of $B_\perp$ around a loop $C(B_\perp(t))$ leads to a geometric phase $\gamma(C, \omega_0)$.

The resulting geometric phase occurs together with the much larger rotation, proportional to the time, due to ordinary precession. It can be isolated by beating the precession signal against a fixed-frequency signal. Notice that this phase depends on ω_0, so that the apparent splitting of nearby resonance peaks ω_0 and ω_0' will be altered by an amount

$$\omega_0 - \omega_0' = \frac{\gamma(C, \omega_0) - \gamma(C, \omega_0')}{T}.$$

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